

5-Chloro-2-methyl-3(2H)-isothiazolone

Other names:	3(2H)-Isothiazolone, 5-chloro-2-methyl-4-Isothiazolin-3-one, 5-chloro-2-methyl-5-Chloro-2-methyl-4-isothiazolin-3-one 2,3-Dihydro-2-methyl-3-oxo-5-chloroisothiazole 5-chloro-2-methyl-2H-isothiazol-3-one
Inchi:	InChI=1S/C4H4ClNOS/c1-6-4(7)2-3(5)8-6/h2H,1H3
InchiKey:	DHNRXBZYEK SXIM-UHFFFAOYSA-N
Formula:	C4H4ClNOS
SMILES:	Cn1sc(Cl)cc1=O
Mol. weight [g/mol]:	149.60
CAS:	26172-55-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.62		Crippen Method
logp	1.100		Crippen Method
mcvol	92.200	ml/mol	McGowan Method
rinpol	1226.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26172554&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

rinpol: Non-polar retention indices

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